

FLOW DIAGNOSTICS, CHEMICALLY  
REACTING TURBULENT FLOW  
MODELING  
AND  
TURBULENT MIXING

A SUMMARY OF PROJECT  
STUDIES IN COMBUSTION

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(NASA-CR-197348) FLOW DIAGNOSTICS,  
CHEMICALLY REACTING TURBULENT FLOW  
MODELING AND TURBULENT MIXING: A  
SUMMARY OF PROJECT STUDIES IN  
COMBUSTION (Cleveland State Univ.)  
130 p

N95-24022

Unclass

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## PUBLICATIONS

## EXPERIMENTAL

- o FLOW VISULIZATION

- o LDV

## SIMULATIONS

- o STRAIGHT VS CURVED

## KINETICS MODELING ( $\text{NO}_x$ )

- o TURBULENT MIXING MODEL FOR  $\text{O}_2$

- o MAXIMUM MIXEDNESS MODEL

**A NUMERICAL SIMULATION OF THE  
EFFECTS OF POSITION AND SPRAY  
OF THE FUEL INJECTION NOZZLE  
ON MIXING IN A CIRCULAR  
COMBUSTOR**

**Bahman Ghorashi and Sastry Taruvai  
Chemical Engineering Department  
Cleveland State University  
Cleveland, Ohio 44115**

**6th Miami International Symposium on Heat and Mass Transfer**

## Optimum Baffle

Baffle (Ht/Wth) = 0.83

Percent of Combustor

Diameter = 35.5

# **NUMERICAL SIMULATION OF FLOW AND THE EFFECT OF BAFFLE ARRANGEMENT ON PRESSURE DROP AND TEMPERATURE PATTERN IN A CIRCULAR COMBUSTOR**

**Bahman Ghorashi and Sastry Taruvai  
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Cleveland State University  
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**8th International Conference on Mathematical and  
Computational Modeling**

## **CONCLUSIONS**

- The optimum baffle size should be about 2.5 inches in height for a 3.0 inch base baffles
- The "out-of -phase" arrangement of baffles is more desirable than "in-phase" arrangement

# FLOW VISUALIZATION AND COMPUTATIONAL STUDIES OF A REVERSE FLOW COMBUSTOR

B. Ghorashi, F. Reardon, G. McBeath  
and  
K. Chun

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Cleveland State University  
Cleveland, Ohio 44115

32nd Heat Transfer and Fluid Mechanics Institute

# **CONCLUSIONS**

- **The temperature distribution becomes relatively uniform as the fuel spread angle increases**
- **The overall effect of the injector position on mixing was not very apparent. Certain patterns were observed, nonetheless, additional optimization studies are needed**



**PROCEEDINGS OF THE  
32nd HEAT TRANSFER AND  
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**Held at  
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June 6 & 7, 1991**

**Edited by  
Frederick H. Reardon  
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Department of Mechanical Engineering**

**School of Engineering and Computer Science  
California State University, Sacramento  
Sacramento, California**

## CONCLUSIONS

- o PATTERN DEPICTED BY SMOKE VISUALIZATION WAS DESIRABLE FOR RAPID MIXING OF FUEL AND AIR
- o MORE EFFECTIVE ATOMIZATION OF FUEL IS REQUIRED
- o LOW INJECTION VELOCITY AND LARGE SPRAY ANGLE PRODUCED A MORE UNIFORM TEMPERATURE DISTRIBUTION AT EXIT

805

## FLOW VISUALIZATION AND COMPUTATIONAL STUDIES OF A REVERSE FLOW CIRCULAR COMBUSTOR

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### ABSTRACT

Computational Fluid Mechanics Studies using the Fluent computer program and flow visualization studies were undertaken to support the development of a reverse-flow circular combustor design. The reverse-flow circular combustor combines a circular geometry with multiple fuel injection nozzles in Mini-Combustion Zones (MCZ). An overall combustor model was developed and used to determine the effects of fuel injector design on the temperature distribution throughout the combustor, with particular attention to the combustor exit. Low injection velocity and large injection spray angle were found to produce a more uniform temperature distribution at the exit.

The flow pattern depicted by the smoke visualization technique showed a behavior which is very desirable for the rapid mixing of fuel and air. The atomization of fuel was visualized by injection of a yellow dye smoke in the liquid side of the air-blast injector. The portion of the combustor volume that was investigated consisted of four baffles on the outermost circular surface and two baffles on the innermost surface. The flow exhibited a rapid circulation pattern inside the MCZs. The channel flow also exhibited a high degree of interaction with the MCZs. Experimental investigation of the flow pattern in the combustor showed similarities to the computational fluid dynamic results.

### INTRODUCTION

The development of efficient air-breathing jet propulsion engines that produce low levels of pollutants in the exhaust will require an improved understanding of the flow and reaction processes that take place in combustion chambers. These processes include atomization and vaporization, when liquid fuels are used, and transport, mixing, and chemical reaction, for both liquid and gaseous fuels. Computational fluid mechanics is a technique for studying these processes without the need for excessive experimental runs.

A flow visualization study of the mixing pattern in a reverse flow combustor was conducted (Figure 1). A transparent model was constructed to examine the flow pattern and mixing of side-mounted turbulent jets and their interaction with the main channel flow. The portion of the combustor volume that was investigated consisted of

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A THERMAL NO<sub>x</sub> PREDICTION MODEL:  
SCALAR COMPUTATION MODULE FOR CFD CODES WITH FLUID AND KINETIC EFFECTS

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ABSTRACT

A model was developed to interface with a CFD, k- $\epsilon$  based code. A converged solution from the CFD code is the input to the post-processing model for prediction of thermal NO<sub>x</sub>. The model uses a decoupled analysis to estimate the equilibrium level of (NO<sub>x</sub>)<sub>e</sub> which in turn is used to predict its rate of formation, (dNO<sub>x</sub>/dt)<sub>e</sub>, at each node. The rate is fixed in the NO<sub>x</sub> production rate plot by estimating the time to reach equilibrium, (t)<sub>eq</sub>, by a differential analysis based on the reaction:  $O + N_2 \rightarrow NO + N$ . The rate is integrated in the non-equilibrium time space based on the residence time at each node in the computational domain. The sum of all nodal predictions yields the total NO<sub>x</sub> level from the combustor. Advantages of this model include: (1) use of all parametric variables of interest for optimization (T, P, N<sub>2</sub>, O<sub>2</sub>, NO<sub>e</sub>,  $\mu$ ,  $P$ ,  $c_{ke}$ ,  $V_m$ ,  $d_n$ ,  $N_{re}$ ,  $De_f$ ,  $\lambda_o$ , A), (2) turbulent mixing effects, (3) geometric effects, (4) lean-to-rich burn combustion conditions, and (5) the potential to work with most k- $\epsilon$  based CFD codes.

## **A COMPARISON STUDY OF STRAIGHT AND CIRCULAR TUBE COMBUSTORS**

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**Kue Chun**  
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### **ABSTRACT**

A Numerical study was conducted using a CFD, k-e based code [ ]. The objective of the study was to compare two combustor configurations i.e., a straight tube combustor and a reverse-low circular combustor. Each of these geometries were further subdivided into one containing the concept of Mini-Combustion-Zones (MCZ) and the other without any compartmentization. The model with MCZ's contained internal baffles and multiple fuel injection ports. The other model contained only a series of multiple injection ports. A one-to-one comparison was made between straight and circular tube combustors with and without MCZ's. The objective was to identify a geometry that could provide complete and immediate combustion of fuel by using the entire combustor space as well as a uniform temperature at the exit of the combustor. The uniformity of temperature was used as a measure of the goodness of mixing.

### **INTRODUCTION**

A COMPARISON OF FLOW VISUALIZATION EXPERIMENTS WITH  
COMPUTATIONAL FLUID DYNAMIC SIMULATIONS OF A CIRCULAR  
COMBUSTOR WITH MINI-COMBUSTION ZONES

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ABSTRACT

Flow visualization experiments were performed to study the nature of complex flow pattern in a circular combustor containing mini-combustion zones (MCZs). The MCZs were structured by bell-shaped baffles located along the inner walls. The premise was that a series of baffles placed along the wall of the combustor could enhance mixing and better utilize the combustor volume. Complex flow patterns were visualized and were photographed with a high speed camera. The results were analyzed and compared to computational fluid dynamic predictions from the Fluent code [1]. The simulations were performed at idle and cruise conditions.

The flow visualization studies examined the mixing effects of two air-blast nozzle designs. One nozzle was a standard expanding turbulent jet atomizer and the other was an air-blast atomizer for turbine engines with a 45 degree swirl vane generating 20 to 60 micron droplets. Using the uniformity of temperature as an indirect measure of goodness of mixing, it was determined that a combustor with mini-combustion zones has definite advantages over a straight-through combustor. Idle and cruise conditions showed similar results in flow pattern in the range of  $M = 0.1$  to  $1.0$  as determined by simulations.

This study also examines the interaction of the airblast nozzle in the mini-combustion zone (MCZ) with the main channel flow. Rapid mixing of combustion products with the main channel flow and the minimization of temperature non-uniformity would minimize  $\text{NO}_x$  generation. The results show a mechanism of mixing which is conducive to reducing nitric oxides in turbine combustors.

**OPTIMIZATION STUDIES OF A REVERSE FLOW CIRCULAR  
COMBUSTOR WITH MCZ'S**

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and

**Kue Chun**  
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**ABSTRACT**

A numerical study was conducted using a CFD, k-e based code [ ]. The objective of the study was to optimize the design of a reverse flow circular combustor [ ]. The circular combustor combines a circular geometry with multiple fuel injection nozzles in the Mini-Combustion-Zones (MCZ). The concept of MCZ's was incorporated by having a series of injection ports and baffles, figure [ ], whereby each injection nozzle and its surrounding baffles would comprise an MCZ.

An overall combustor model was developed and was used to determine the effects of nozzle position, fuel spray angle, baffle positions with respect to each other, number of baffles, dimensions of baffles and the location of baffles. Initially the baffles were placed on top and bottom surfaces of the combustor and the optimization studies were performed [ ]. Industrial constraints were later introduced into the design and further studies were performed with baffles placed only on one side. The objective of this study was then to compare these two final design configurations and determine which of these geometries could provide the requirements such as low pressure drop within the combustor, uniform temperature at the exit of the combustor (a measure of goodness of mixing), as well as complete and immediate combustion of fuel by using the entire combustor space.

**A NUMERICAL SIMULATION OF THE EFFECTS OF POSITION AND  
SPRAY ANGLE OF THE FUEL INJECTION NOZZLE  
ON MIXING IN A CIRCULAR COMBUSTOR**

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**Chemical Engineering Department**

**Cleveland State University**

**Cleveland, Ohio 44115**

**ABSTRACT**

A Numerical study was conducted using Fluent computer program developed by Creare, Inc. The objective was to determine the flow pattern between two sets of baffles in an experimental reverse-flow circular combustor, designed for enhanced mixing and NO<sub>x</sub> reduction, by varying the position and spray angle of the fuel injection nozzles. The segment of the combustor that was investigated consisted of two baffles positioned on the upperface and two on the lowerface of the circular combustor. Heated air at 300°F and 3 atmospheres pressure was introduced into the combustor with an inlet velocity of 100 ft/sec. The fuel, pentane, was introduced into the main stream via fuel injection nozzles. There were four nozzles, two on the upper and two on the



NUMERICAL SIMULATION OF FLOW AND THE EFFECT OF BAFFLE  
ARRANGEMENT ON PRESSURE DROP AND TEMPERATURE PATTERN  
IN A CIRCULAR COMBUSTOR

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ABSTRACT

A numerical simulation study was conducted to determine the effect of baffle arrangement on pressure drop in an experimental reverse-flow circular combustor with several Mini-combustion Zones (MCZ). The Fluent computer code developed by Creare Inc., was used for this study. Three parameters which appeared to significantly affect the pressure drop were varied, and pressure drop for each case was numerically determined. The portion of the combustor volume that was investigated had two baffles on the upper face and two baffles on the lower face. Heated air at 1000°F with an inlet air velocity of 100 ft/sec and 1 atmosphere pressure was introduced into the combustor. Fuel (pentane) at 80°F was introduced via nozzles which were placed between the baffles. The following changes were then made in the baffle arrangement and the effects on the pressure drop and temperature distribution were evaluated for each of the following cases:

1. The positions of the baffles on the upper and lower face were changed.
2. The dimensions of the baffles were varied.
3. The shapes of the baffles were altered.

The effects of the above mentioned design alterations are summarized.

KEYWORDS

Mini-combustion-zones; baffles; pressure drop; combustor.

INTRODUCTION

A reverse-flow circular combustor based on the design proposed by Ghorashi [1,2,3] in 1987 was studied. This approach introduces the concept of Mini-Combustion-Zones (MCZ) to use the entire reactor volume via radial injection of fuel along the axial main flow. In addition to this, the use of Mini-Combustion-Zones generates recirculation within the MCZs, making each MCZ to behave like a well-stirred reactor.

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## Summary of LDV Results

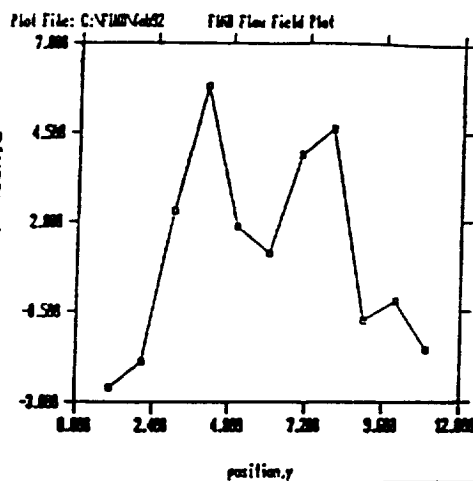
- \* Main flow and nozzle flow mixing is indicated by high turbulence intensity values (peaks) at the same location.
- \* Higher velocities were evident near the inner radius of the combustor.
- \* Multiple high turbulent intensity peaks in the MCZ indicate significant mixing is occurring.
- \* Shear layers from baffle peaks interact with nozzle flow increasing local mixing
- \* Mainflow air adds to the uniformity of mixing across the Y-cross section and enhances the overall mixing in the Y-plane (Area under curve).
- \* Main flow pressure-increases result in higher axial velocity and lower radial velocities.



position,y

Commands:  
Print screen  
Graph menu

FIGURE 2



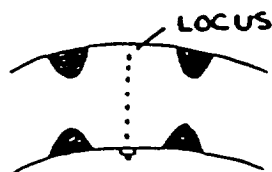
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Plot 2 = 0 :  
Plot 3 = + :  
Plot 4 = x :

Commands:  
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Graph menu

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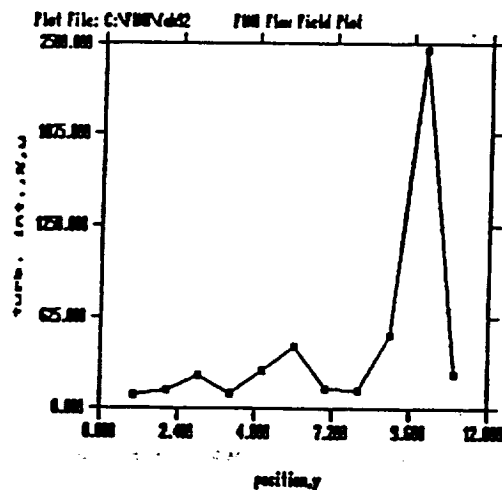


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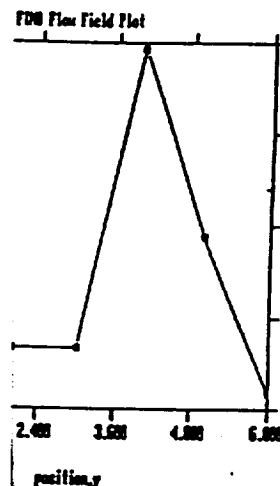
NOZZLE CENTER

FIGURE 4



Plot 1 = 0 :  
Plot 2 = 0 :  
Plot 3 = + :  
Plot 4 = x :

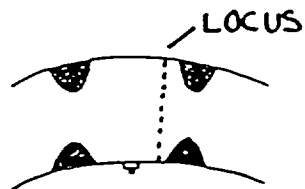
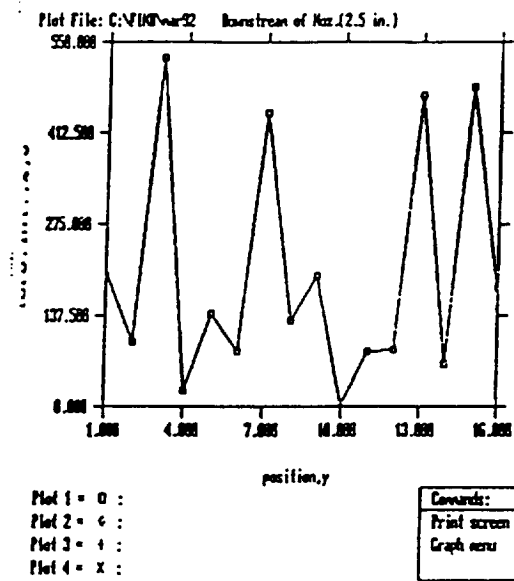
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Commands:  
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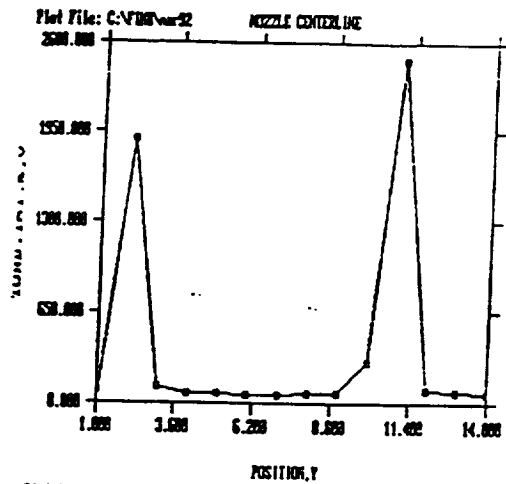
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FIGURE 7



VENTURI ENTRANCE

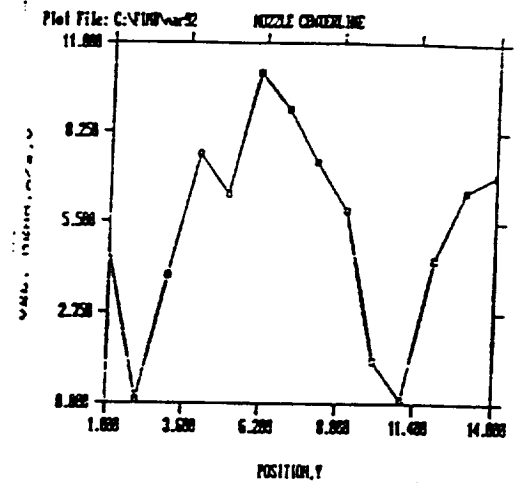
FIGURE 8



Plot 1 = G :  
 Plot 2 = + :  
 Plot 3 = + :  
 Plot 4 = x :

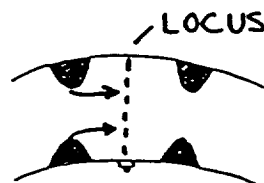
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FIGURE 9



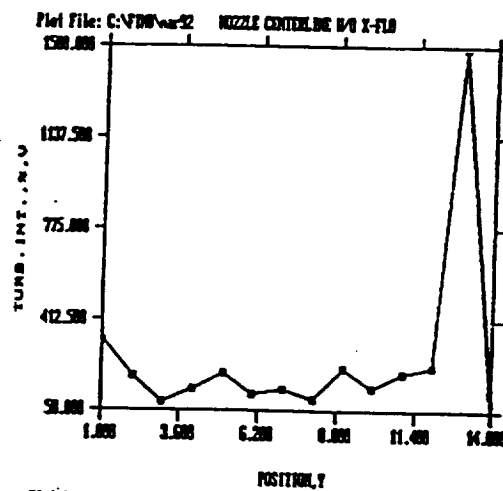
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 Plot 2 = + :  
 Plot 3 = + :  
 Plot 4 = x :

Commands:  
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 Graph menu



NOZZLE CENTER

FIGURE 10

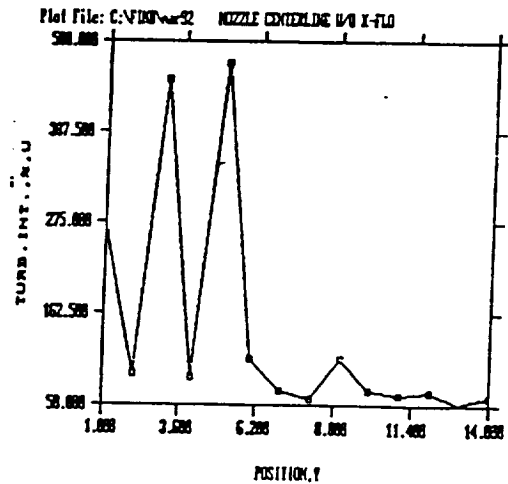


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 Plot 3 = + :  
 Plot 4 = x :

Commands:  
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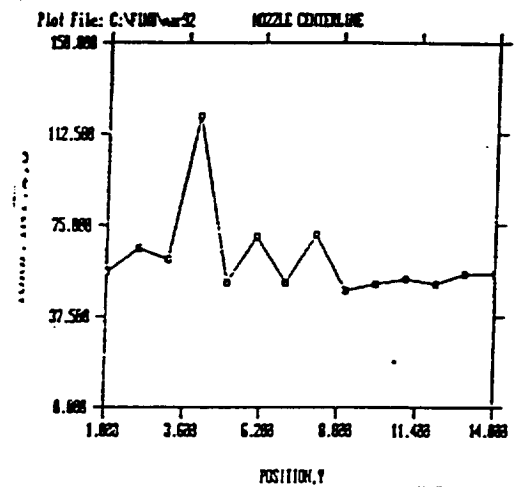
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FIGURE 11

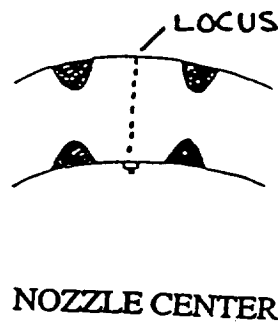


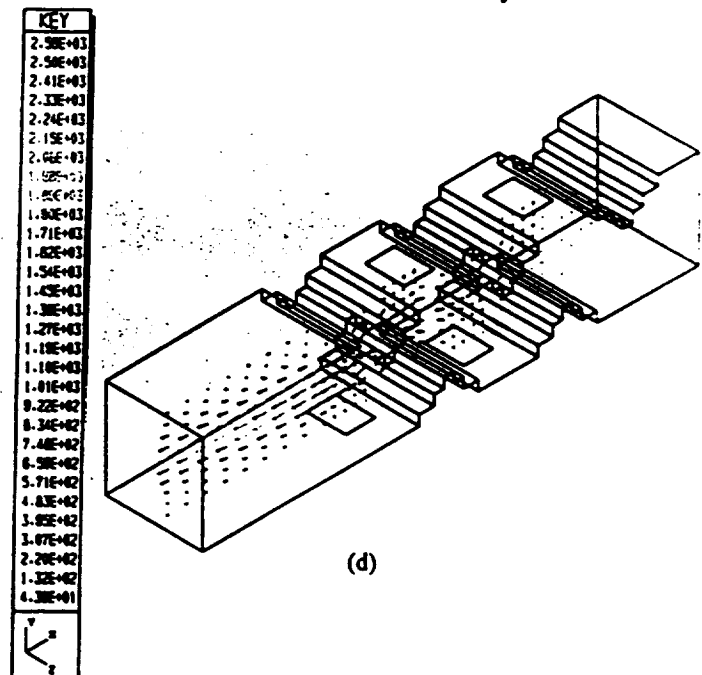
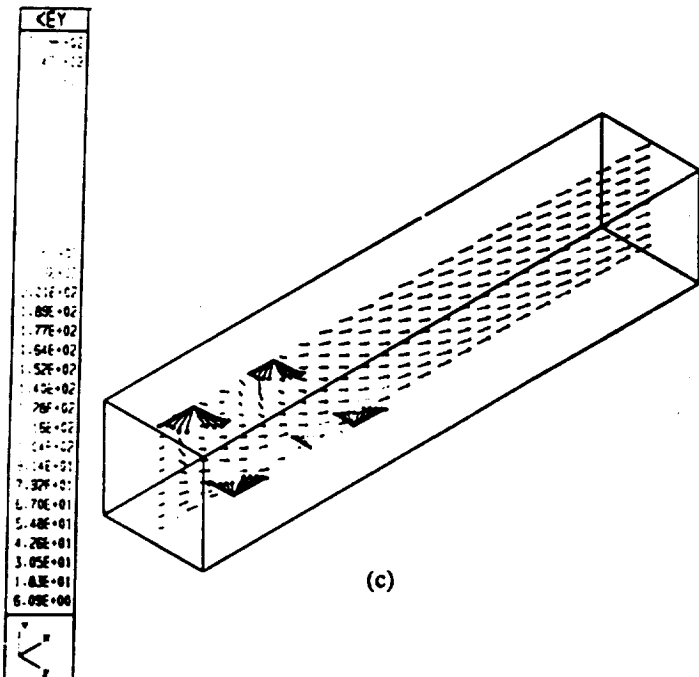
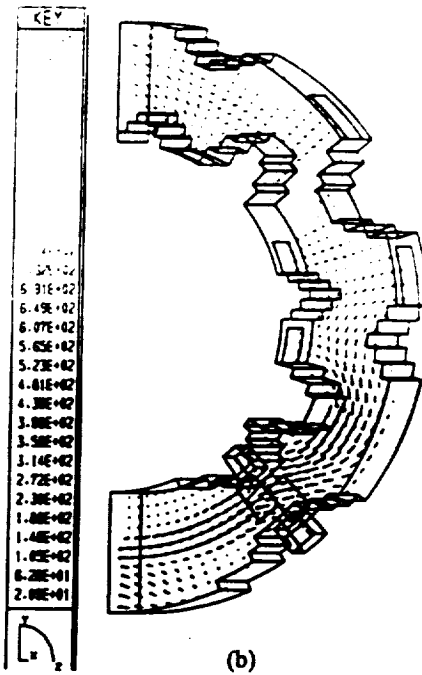
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Plot 3 = + :  
Plot 4 = x :

FIGURE 12

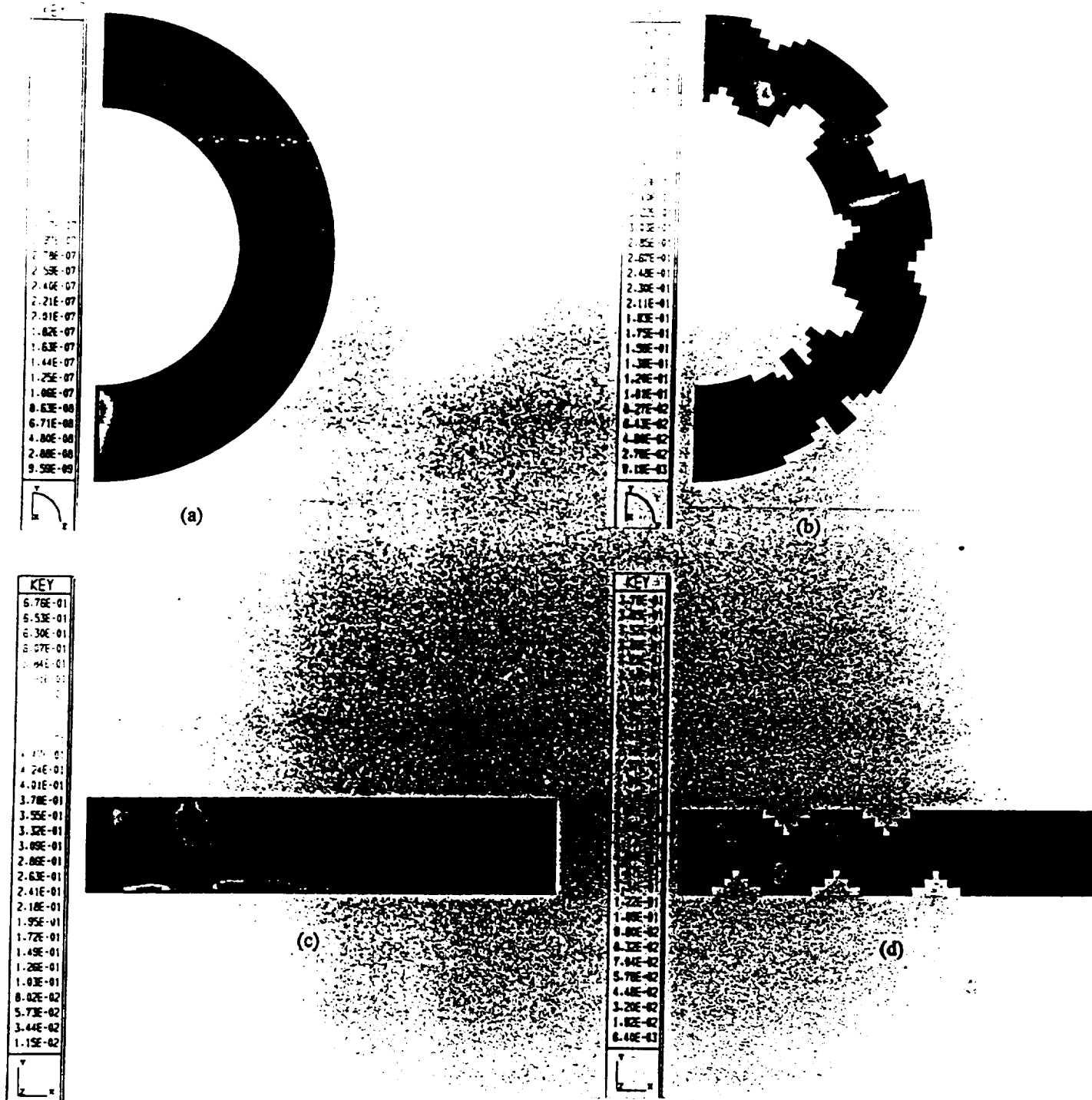


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Plot 3 = + :  
Plot 4 = x :





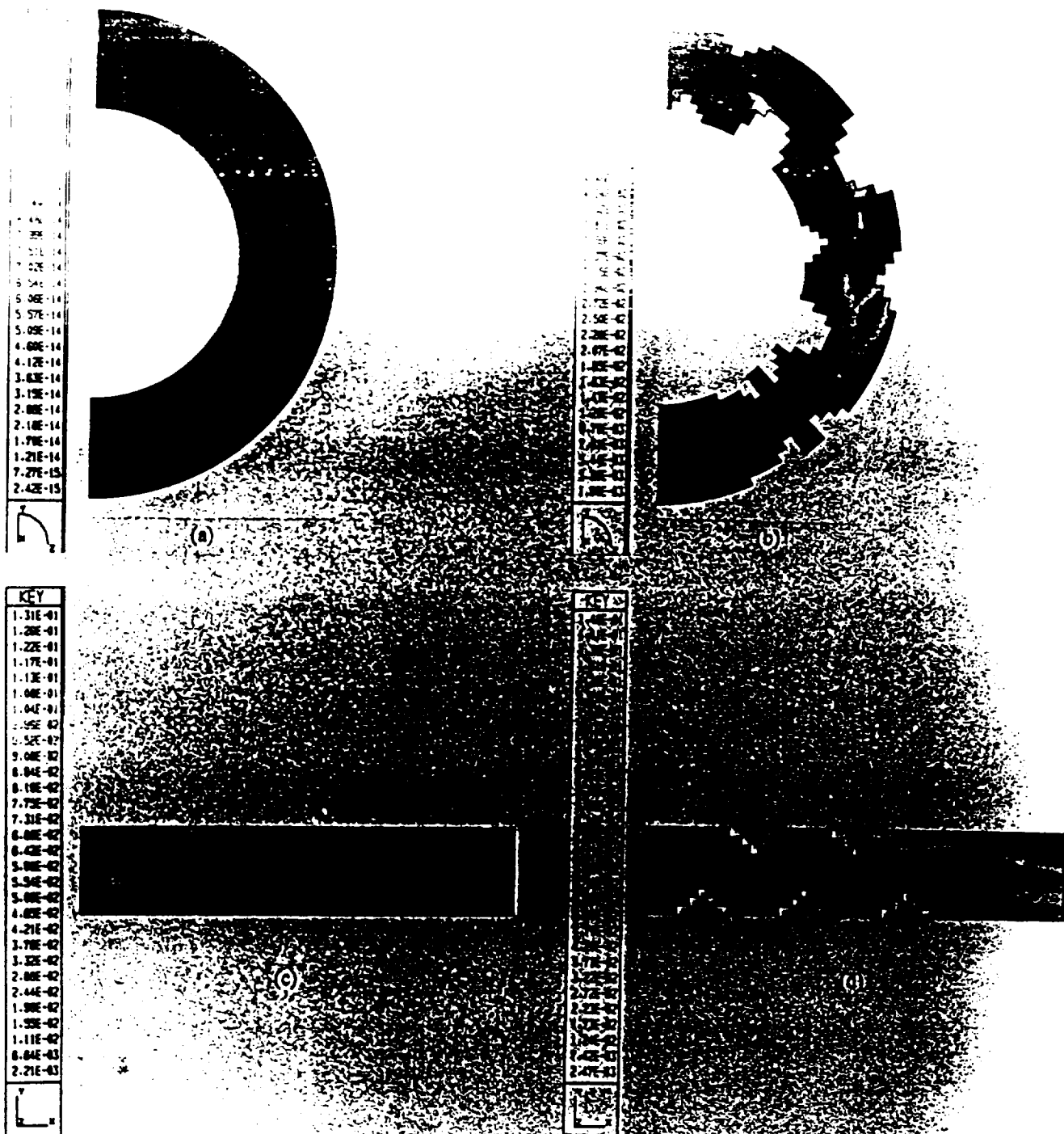
(a) - Circular, no Baffles (b) - Circular, Baffles  
(c) - Straight, no Baffles (d) - Straight, Baffles



COMPARISON OF COMPUTER SIMULATION RESULTS  
FOR C8H18 MASS FRACTION  
MASS FRACTION DIMENSIONLESS  
ORIENTATION X, PALNE 6, 3 - D DOMAIN

(a) - Circular, no Baffles (b) - Circular, Baffles  
(c) - Straight, no Baffles (d) - Straight, Baffles

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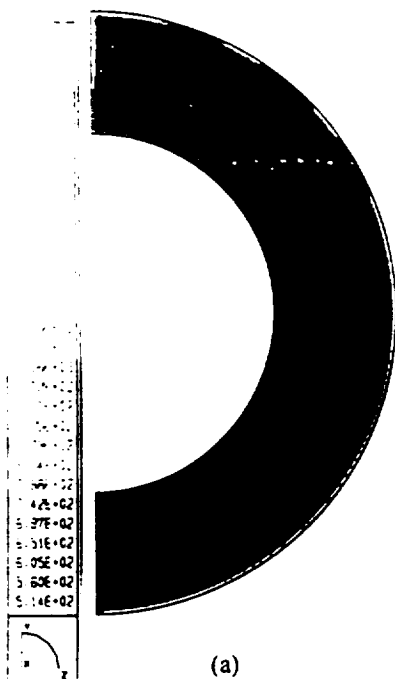


COMPARISON OF COMPUTER SIMULATION RESULTS  
FOR CO MASS FRACTION  
MASS FRACTION DIMENSIONLESS  
ORIENTATION X, PALNE 6, 3 - D DOMAIN

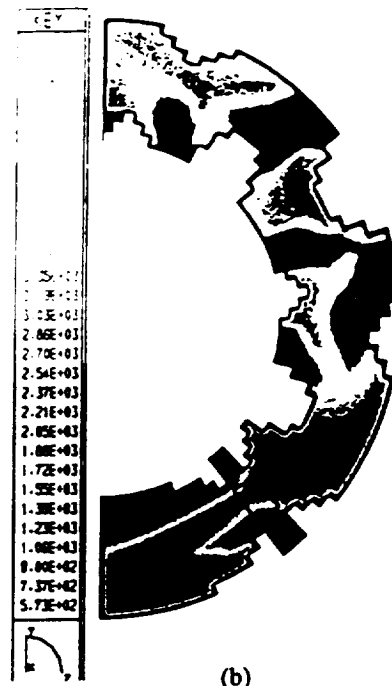
(a) - Circular, no Baffles (b) - Circular, Baffles  
(c) - Straight, no Baffles (d) - Straight, Baffles

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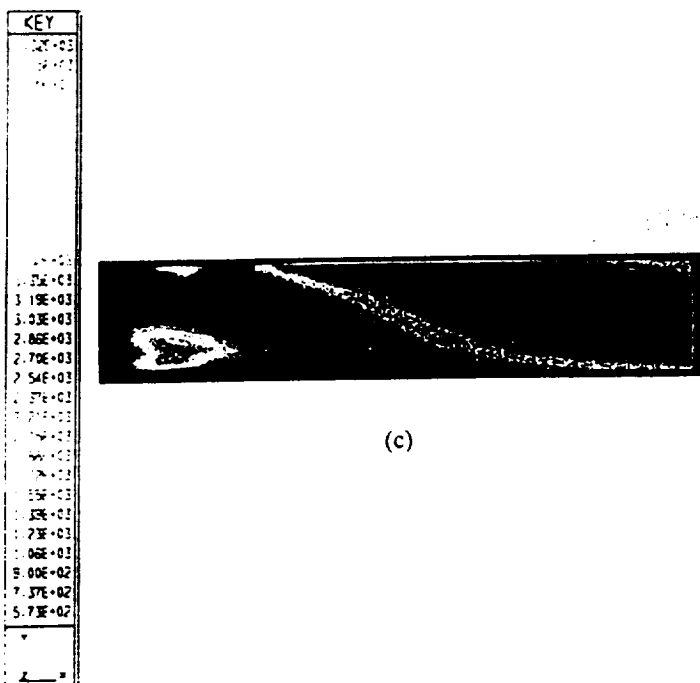




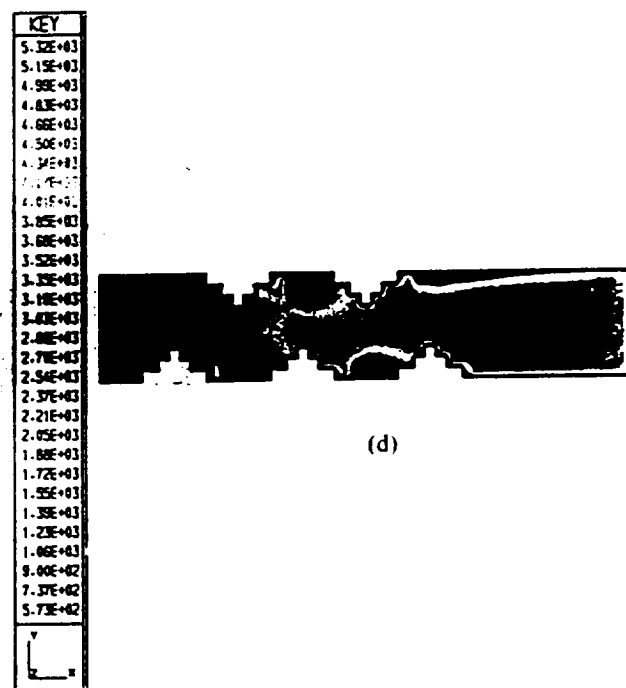
(a)



(b)



(c)

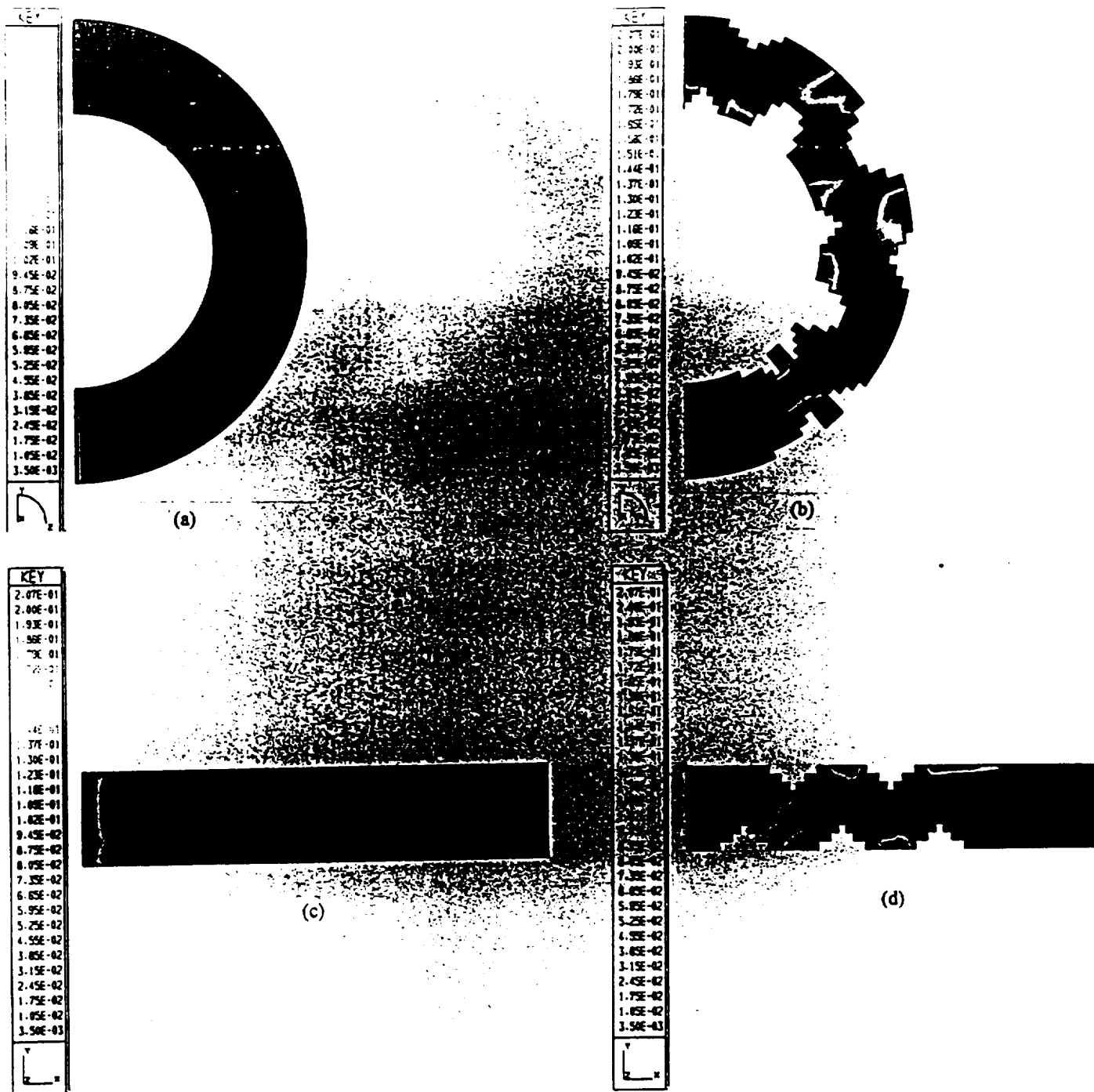


(d)

COMPARISON OF COMPUTER SIMULATION RESULTS  
FOR TEMPERATURE PATTERN  
TEMPERATURE IN DEGREE RANKINE  
ORIENTATION X, PALNE 6, 3 - D DOMAIN

(a) - Circular, no Baffles (b) - Circular, Baffles  
(c) - Straight, no Baffles (d) - Straight, Baffles

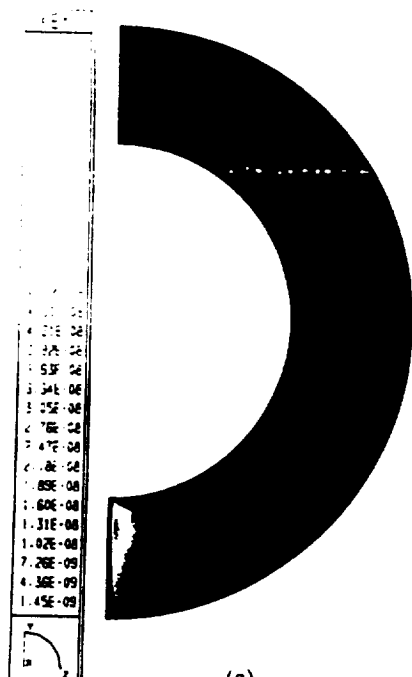
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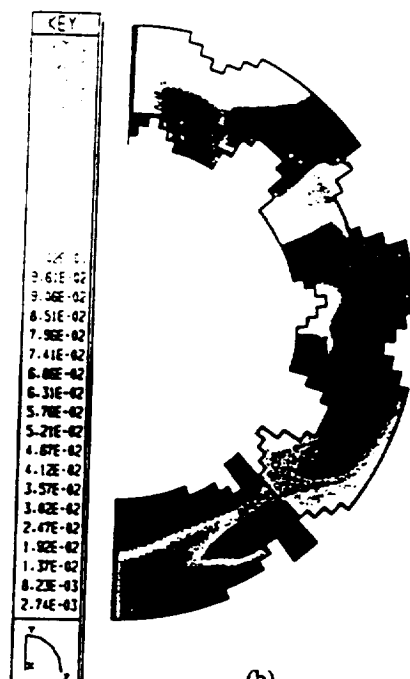
COMPARISON OF COMPUTER SIMULATION RESULTS  
FOR O2 MASS FRACTION  
MASS FRACTION DIMENSIONLESS  
ORIENTATION X, PALNE 6, 3 - D DOMAIN

(a) - Circular, no Baffles (b) - Circular, Baffles  
(c) - Straight, no Baffles (d) - Straight, Baffles

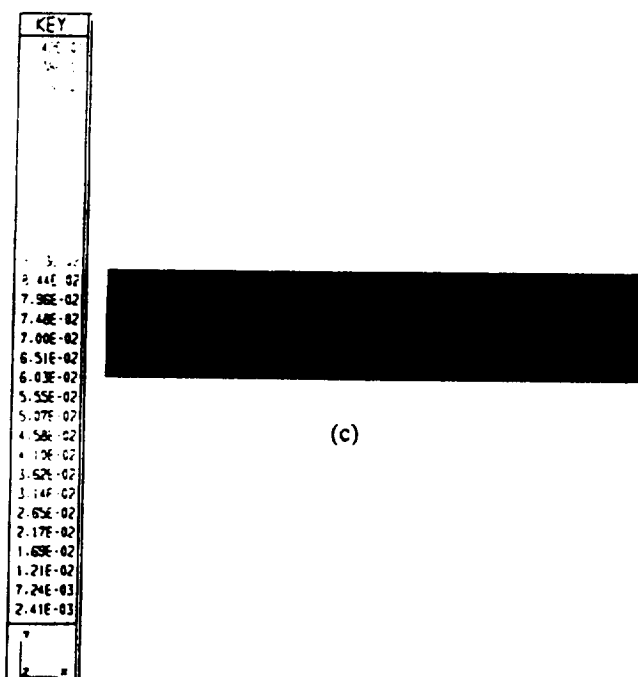
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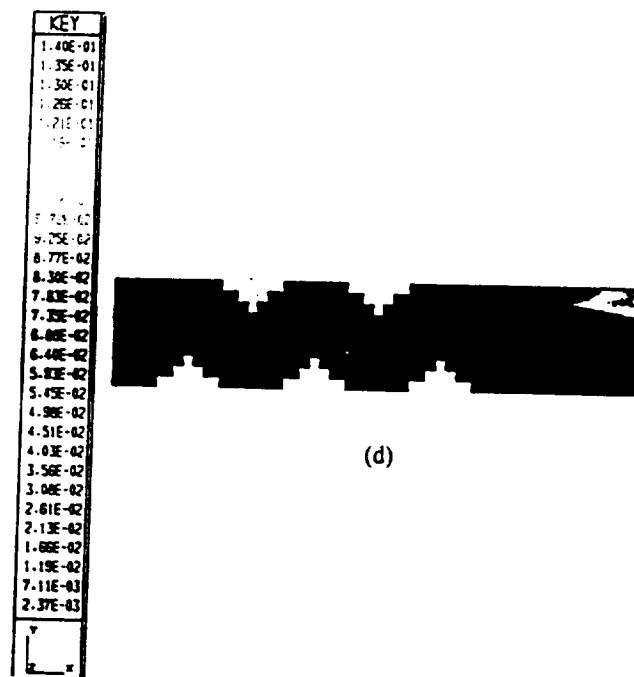
(a)



(b)



(c)



(d)

COMPARISON OF COMPUTER SIMULATION RESULTS  
FOR CO<sub>2</sub> MASS FRACTION  
MASS FRACTION DIMENSIONLESS  
ORIENTATION X, PALNE 6, 3 - D DOMAIN

(a) - Circular, no Baffles (b) - Circular, Baffles  
(c) - Straight, no Baffles (d) - Straight, Baffles

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# **THERMAL NO<sub>x</sub> PREDICTION MODEL**

## **PROCEDURE:**

**Converged Fluent Case (k-epsilon Model)**

### **1. INPUT:**

**Pressure**

**Temperature**

**Oxygen Concentration**

**Nitrogen Concentration**

**Eddy Dissipation**

**Effective Viscosity**

**Density**

**Velocity Magnitude**

2. Calculate Effective Diameter ( $D_e$ ) and the Cross-Sectional Area ( $A_x$ ) of the Combustor at Each Node  
Plane

$$D_e = 4 * \text{Area} / \text{Perimeter}$$

$$A_x = L * W$$

3. Calculate Kolmogorov Length Scale at Each Node

$$\lambda_0 = [(\mu/\rho)^3/\epsilon]^{0.25}$$

4. Calculate Turbulent Reynolds Number at Each Node

$$N_{TE} = [D_e |V_m| \rho / \mu]$$

5. Calculate  $\lambda_{PM}$  at Each Node

$$\lambda_{PM} = \sqrt{(\mu * A / D_e |V_m| \rho)}$$

6. Calculate the Residence Time for Each Node

$$t_{RT} = d / |V_m|$$

7. Test for the Degree of Mixing at Each Node

( If  $0 < \lambda_{PM} / \lambda_0 \leq 1$ , go to step A

if  $\lambda_{PM} / \lambda_0 = 0$ , go to step B)

A. Good Mixing =  $2.78 * [\text{Hung's Eq.}]$  (Smith, et.al.)

B. Diffusion Limited Case =  $1.00 * [\text{Hung's Eq.}]$

**Note:** Correction for Nitrogen Conversion at each Node Might Yield More Accurate Results, However, it would be Computationally Inefficient. Nonetheless, the latter should be tested.

$$[N]_t = 2\beta\gamma t/\alpha + \gamma/\alpha(1 - e^{-\alpha t})$$

**9. Calculate the Equilibrium Values of Oxygen, Nitrogen and Nitric Oxide with 18-Step Octane Combustion Model (Kopa, et.al.)**

$$K_7 = \frac{(C)(O_2)^{1/2}}{(CO)} \quad K_{14} = \frac{(C)(N_2)^{1/2}(E_2)^{1/2}}{(ECN)}$$

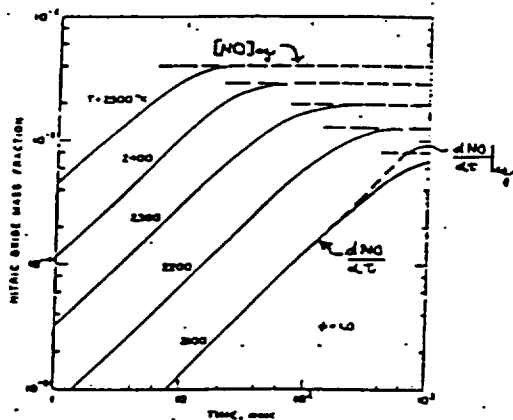
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000
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10. Calculate the Rate of Nitric Oxide Formation at the Intersection of Equilibrium NO and NO Rate-Line, Using the Hung Equation at Each Node

$$dX_{NO}/dt = P^{1/2}[(aX_{N_2}X_{O_2}^{1/2} - bX_{NO}^2/X_{O_2}^{1/2}) / (1 + cX_{NO}/X_{O_2})]$$

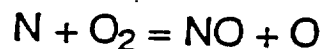
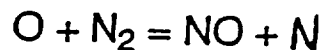
Where a,b,c is determined from the Arrhenious Equation



11. Estimate the Relaxation Time Via the Differential Analysis of the Controlling Mechanism

$$t_{calc} = [NO]_e/2\gamma$$

12. Calculate the Actual Time Based on Two-Step Mechanism



$$t_{RX} = t_{calc}/2$$

13. Construct Semi-Log  $NO_x$  Formation Rate Curves (refer to Step 10)

**14. Determine Non-equilibrium NO<sub>x</sub> Formation Rates**

**Note:** Interpret Curve to Find Non-equilibrium NO Rate at Lower Limit [ $t_{RT} * 0.01$ ] and at Upper Limit [ $t_{RT}$ ].

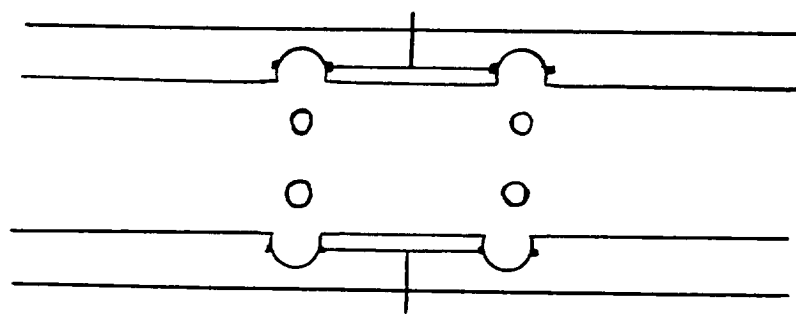
**15. Integrate the Rate with respect to Time**

$$NO(i,j) = \int dNO/dt * dt = 0.5 * (t_{RT} - 0.01 * t_{RT}) * \Delta dNO/dt$$

**16. Sum all the Local NO<sub>x</sub> Values to Estimate the Total Thermal NO<sub>x</sub>**

$$NO_x = \sum_{i,j=1}^m NO(i,j) \text{ for } K = 1 \text{ to } N$$





# ALTERNATE METHOD

## Procedure

Converged FLUENT Case

### 1. INPUT

Pressure

Temperature

Oxygen Concentration

Nitrogen Concentration

Velocity Magnitude

Assume Constant Nitrogen Concentration

### 2 Use Global Forward-Rate Reaction to Estimate the Local NO<sub>x</sub> Formation

$$[\text{NO}] = K e^{(-k_2/T)} [\text{N}_2] [\text{O}_2]^{1/2} t$$

Where [ ] = mole fraction

T = Temperature

t = time

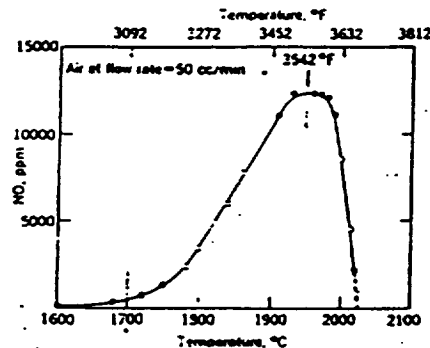
K, K<sub>2</sub> = constants

### 3. Integrate with respect to Residence Time

#### 4. Sum all the Values in order to Obtain the Total Thermal NO<sub>x</sub>

### Limitations of this Method

#### 1. Temperature Range



$$2030^{\circ}\text{C} < T < 1700^{\circ}\text{C}$$

#### 2. Assumptions

$$dX_{\text{NO}}/dt = P^{1/2}[(aX_{\text{N}_2}X_{\text{O}_2}^{1/2} - bX_{\text{NO}}^2/X_{\text{O}_2}^{1/2})/(1 + cX_{\text{NO}}/X_{\text{O}_2})]$$

if  $X_{\text{NO}}$  is small, then  $(X_{\text{NO}})^2 \approx 0$

if  $X_{\text{NO}}$  is small, then  $X_{\text{NO}}/X_{\text{O}_2} \approx 0$

$$[\text{NO}] = K e^{(-k_2/T)} [\text{N}_2] [\text{O}_2]^{1/2} t$$

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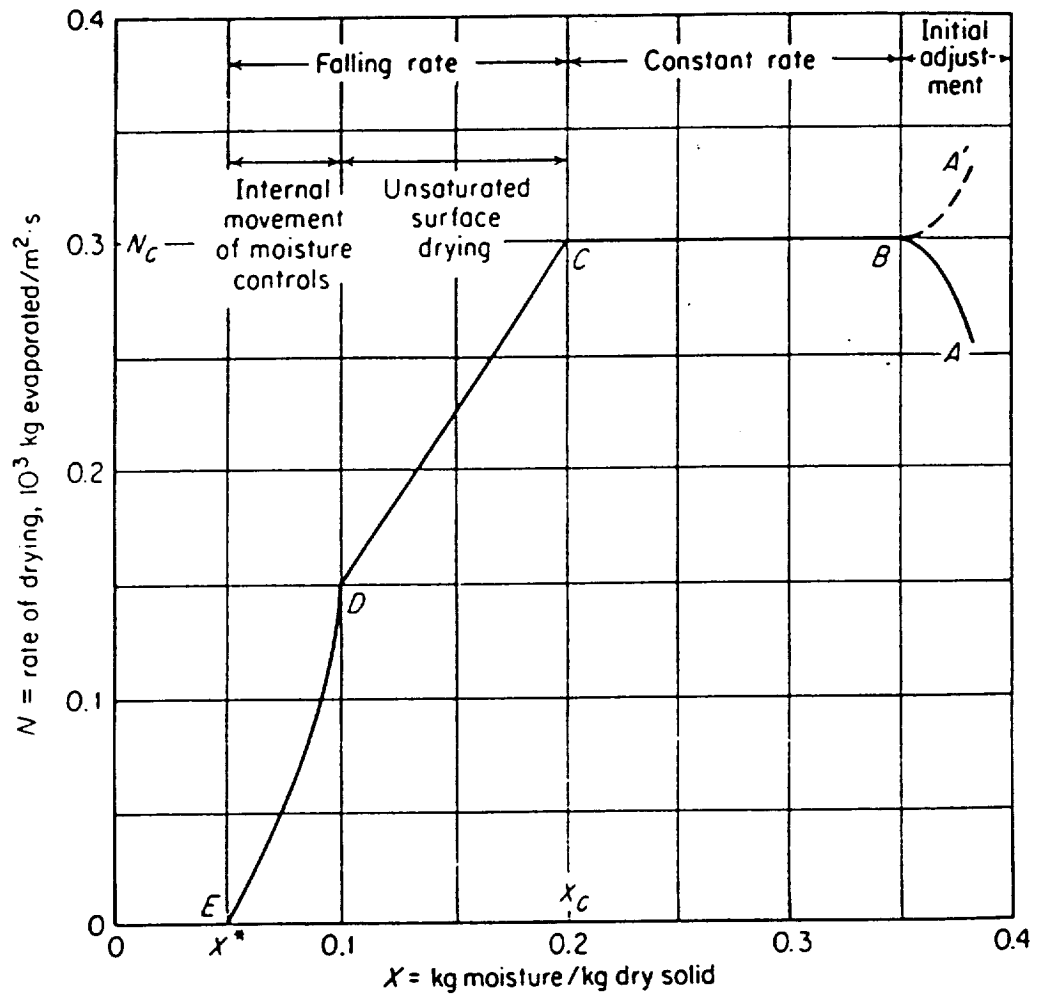


Figure 12.10 Typical rate-of-drying curve, constant drying conditions.

The equivalent molecular diameter is given by equation

$$\sigma = \sqrt{\frac{8.28 \times 10^{-20} T^{1.5\rho}}{\mu P_m^{1/2}}}$$

The mass diffusivity can be calculated from:

$$D = \frac{2.628 \times 10^{-19} \sqrt{T^3/M}}{P \sigma^2}$$

The Schmidt number of air is given by

$$(Sc)_{\text{air}} = \frac{\mu}{\rho D_{AB}}$$

$$(Sc)_{\text{air}} = \frac{\nu}{D_{AB}}$$

For the high-Schmidt-number case, the time constant can be obtained by

$$\tau = \frac{1}{2} \left[ 3 \left( \frac{5}{\pi} \right)^{2/3} \left( \frac{L_i^2}{\epsilon} \right)^{1/3} + \left( \frac{\nu}{\epsilon} \right)^{1/2} \ln N_{Sc} \right]$$

no mixing in the limit of infinite Schmidt number is now satisfied ( $\tau = \infty$ ,  
which gives  $I_s = 1$  for all time).

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The local mixing problem is simplified

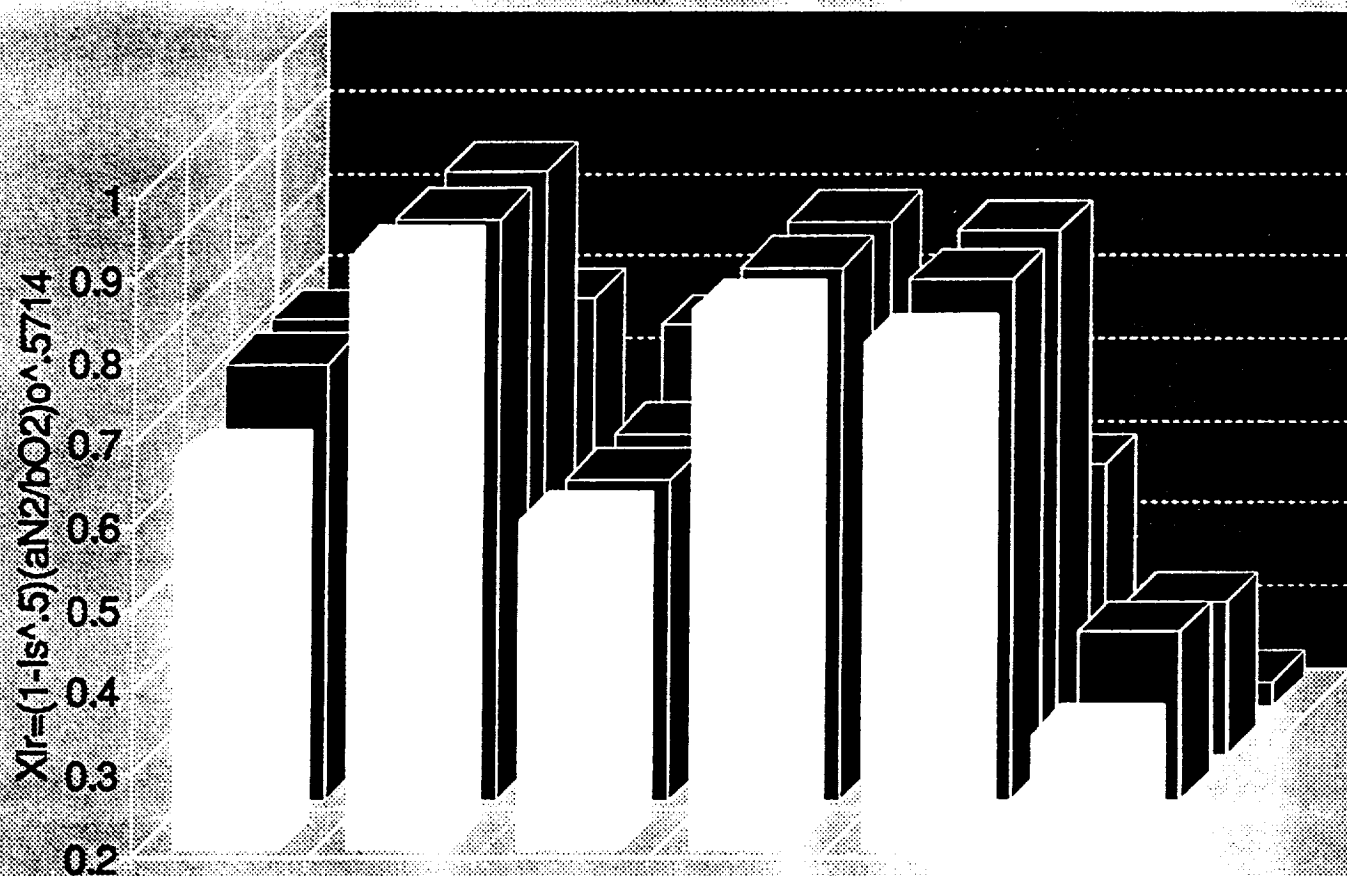
$$I_s = \frac{1}{1 + \tau'/\tau}.$$

Isotropic theory as previously presented could be applied to mixing-vessel problems with some degree of approximation. However, in this case the turbulent field will decay in certain regions of the mixer. Probably the only area which would approximate a constant turbulent field is that in the immediate vicinity of the stirrer.

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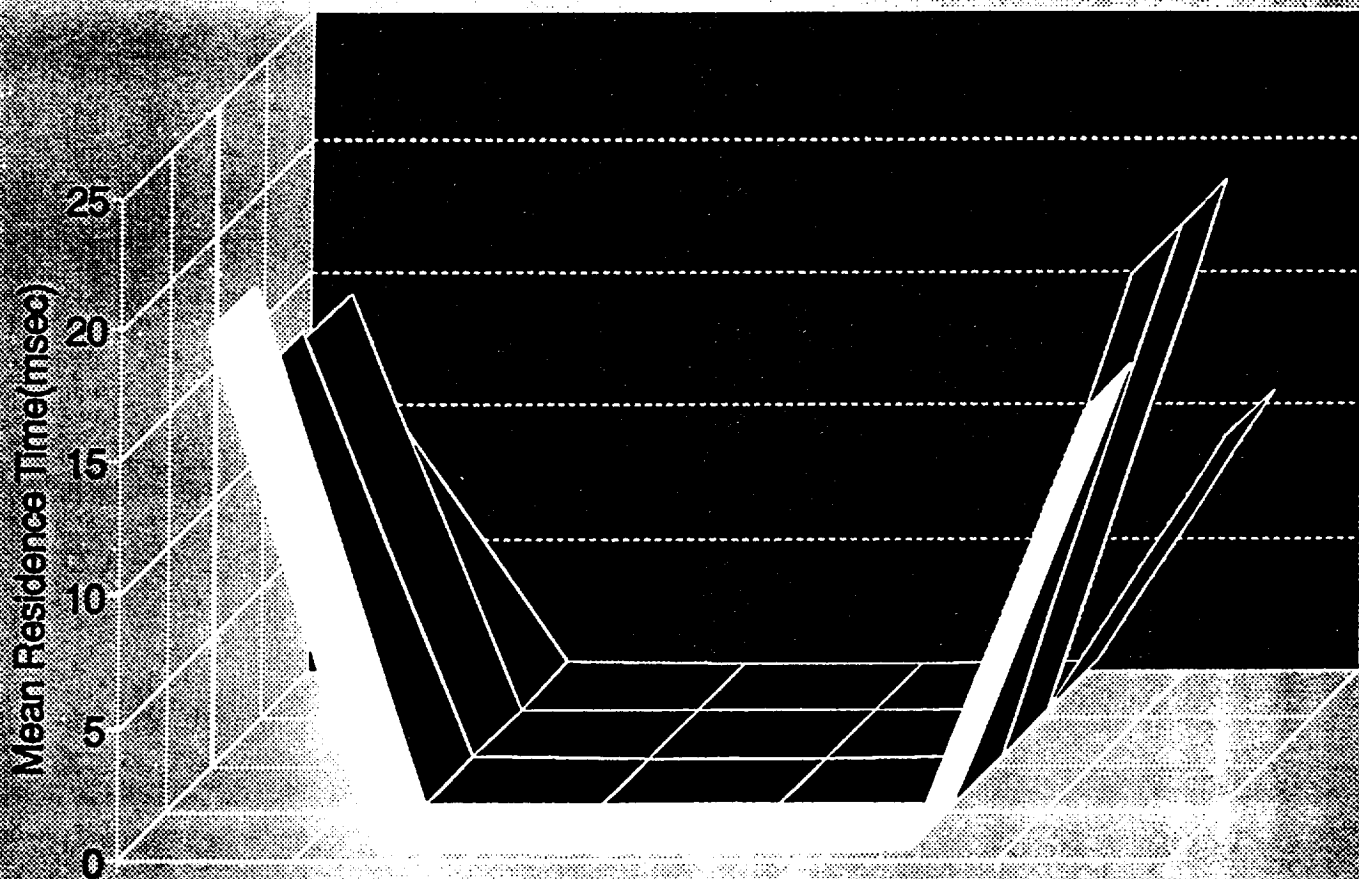
## FRACTION CONVERT. VS MIXING



Position: l=2 to 8 by 2, J=2 to 12 by 2



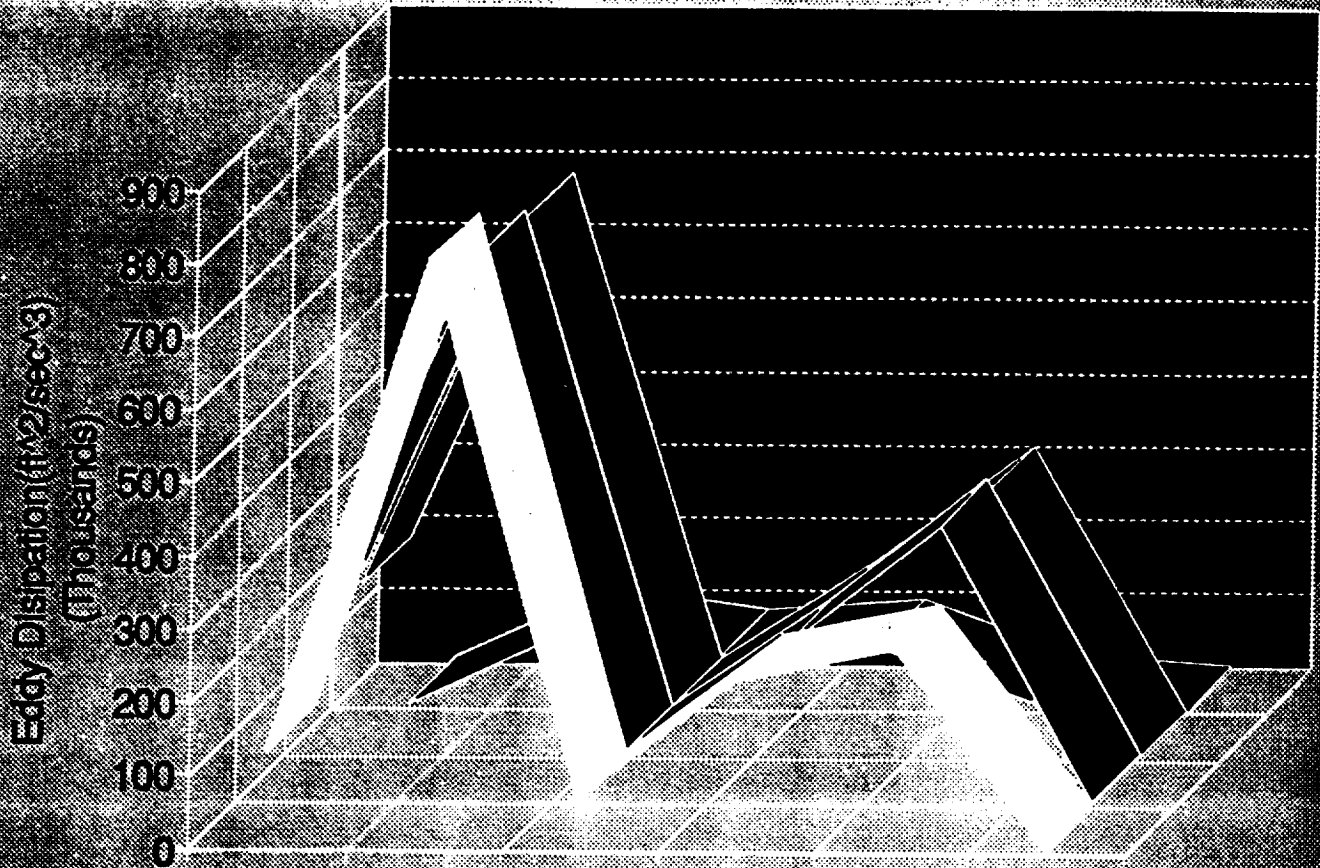
# MEAN RESIDENCE TIME BTWN NODES



Position: I=2 to 8 by 2, J=2 to 12 by 2

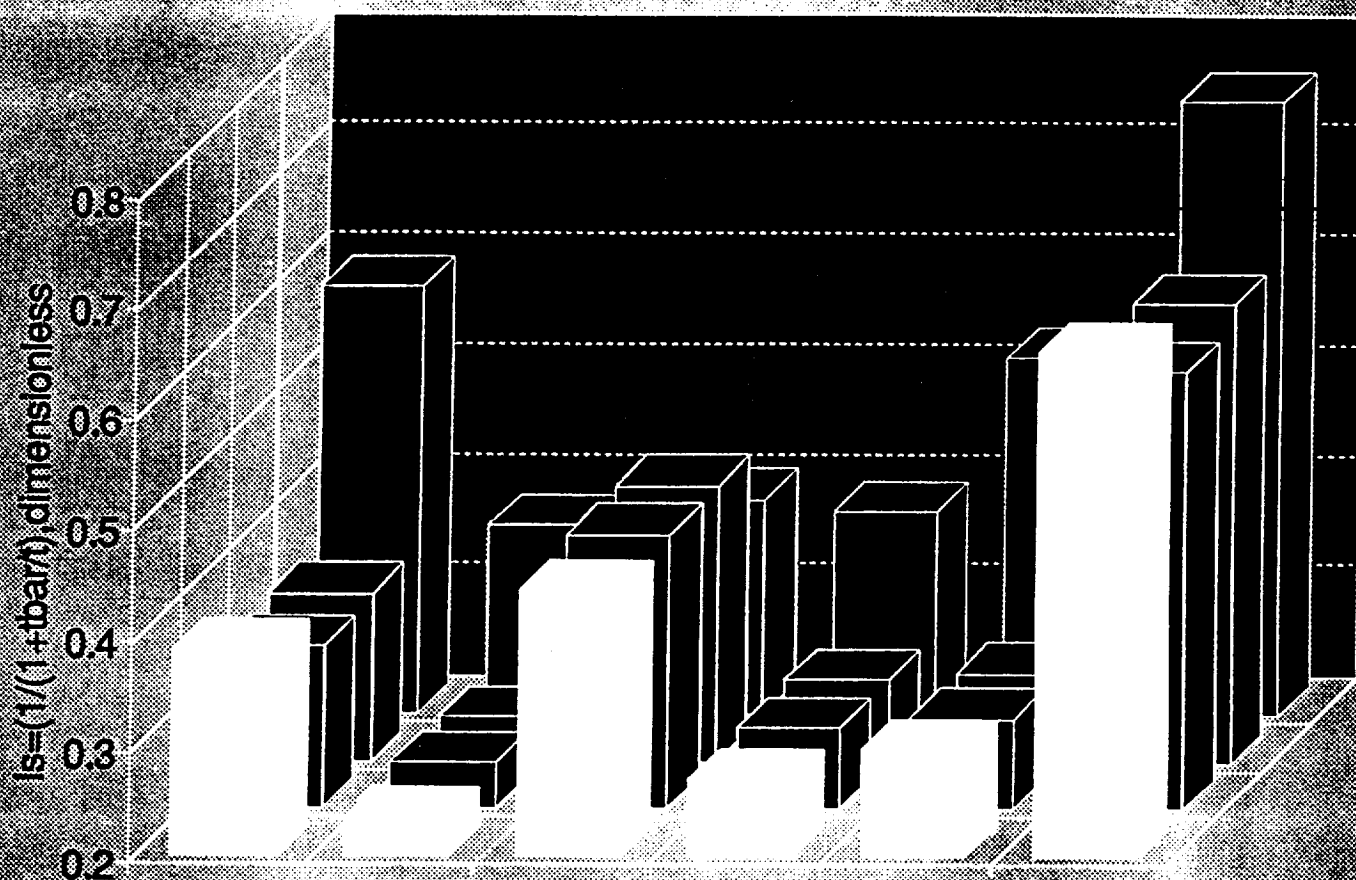
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# EDDY DISSIPATION



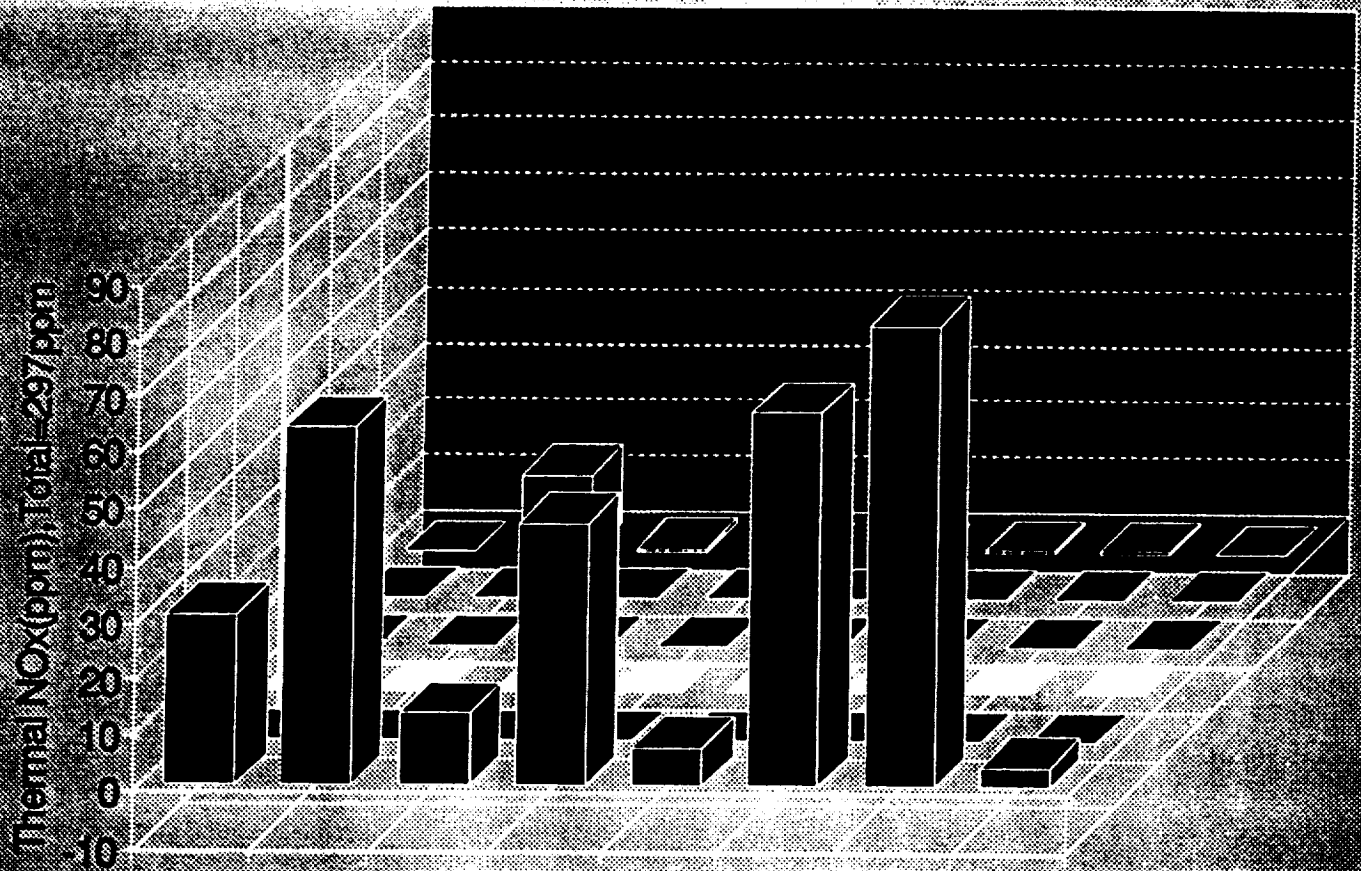
Position: I=2 to 8 by 2, J=2 to 12 by 2

# INTENSITY OF SEGREGATION



Position:  $l=2$  to  $8$  by  $2$ ,  $J=2$  to  $12$  by  $2$

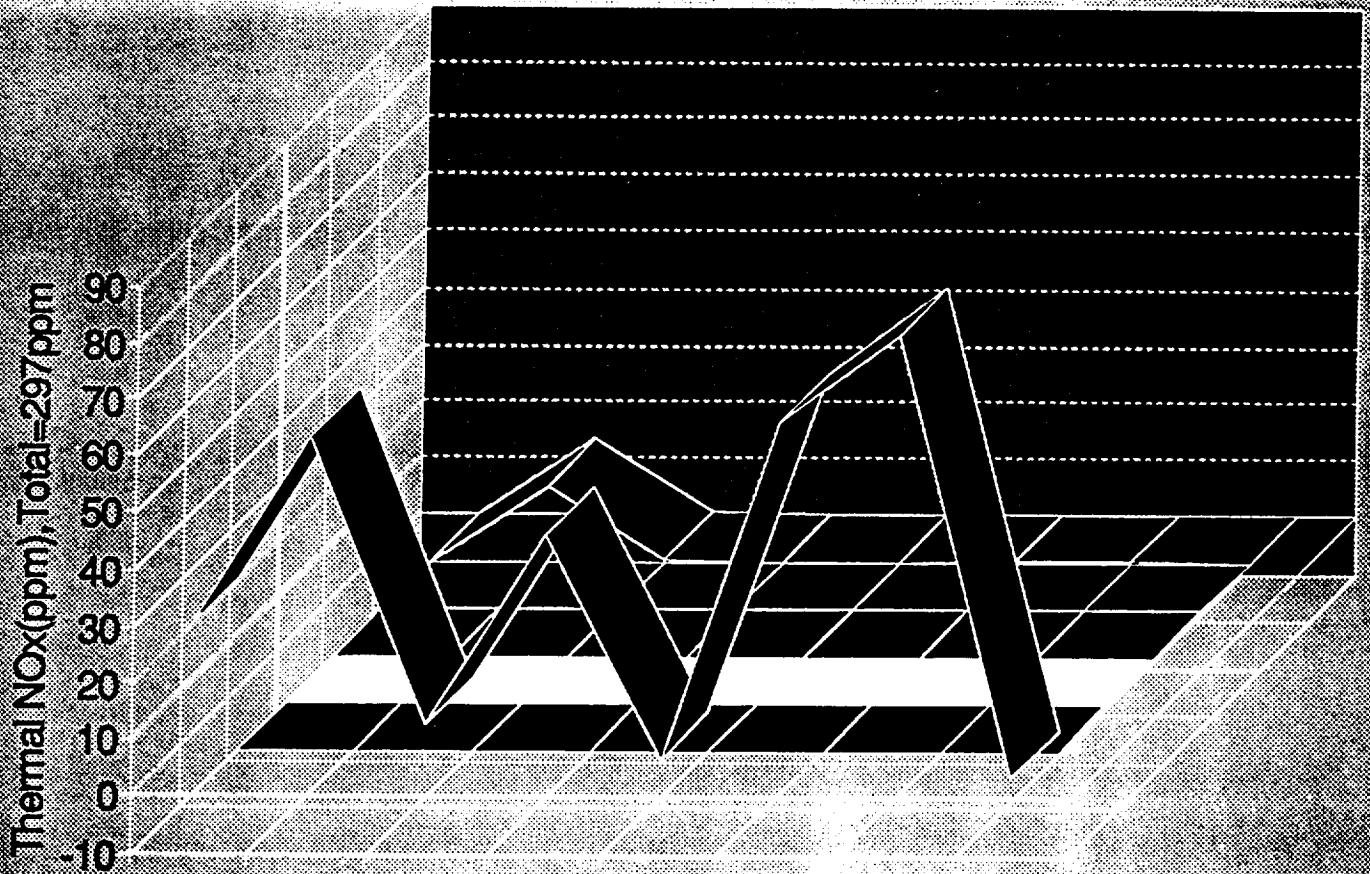
# THERMAL NO<sub>x</sub> PREDICTION



Position: I=2to9, J=4to9, K=10

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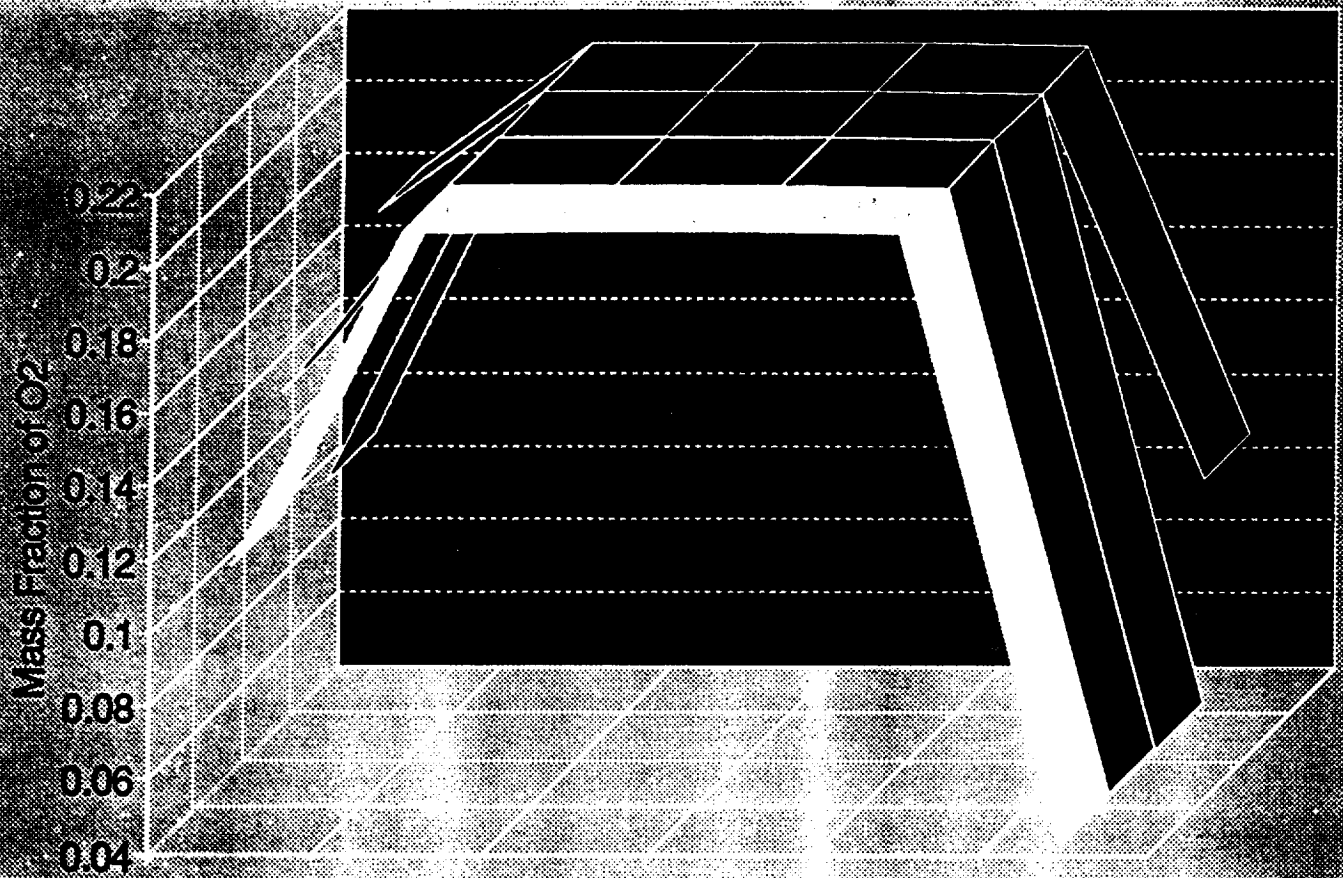
# THERMAL NO<sub>x</sub> PREDICTION



Position: I=2 to 9, J=4 to 9, K=10

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# OXYGEN

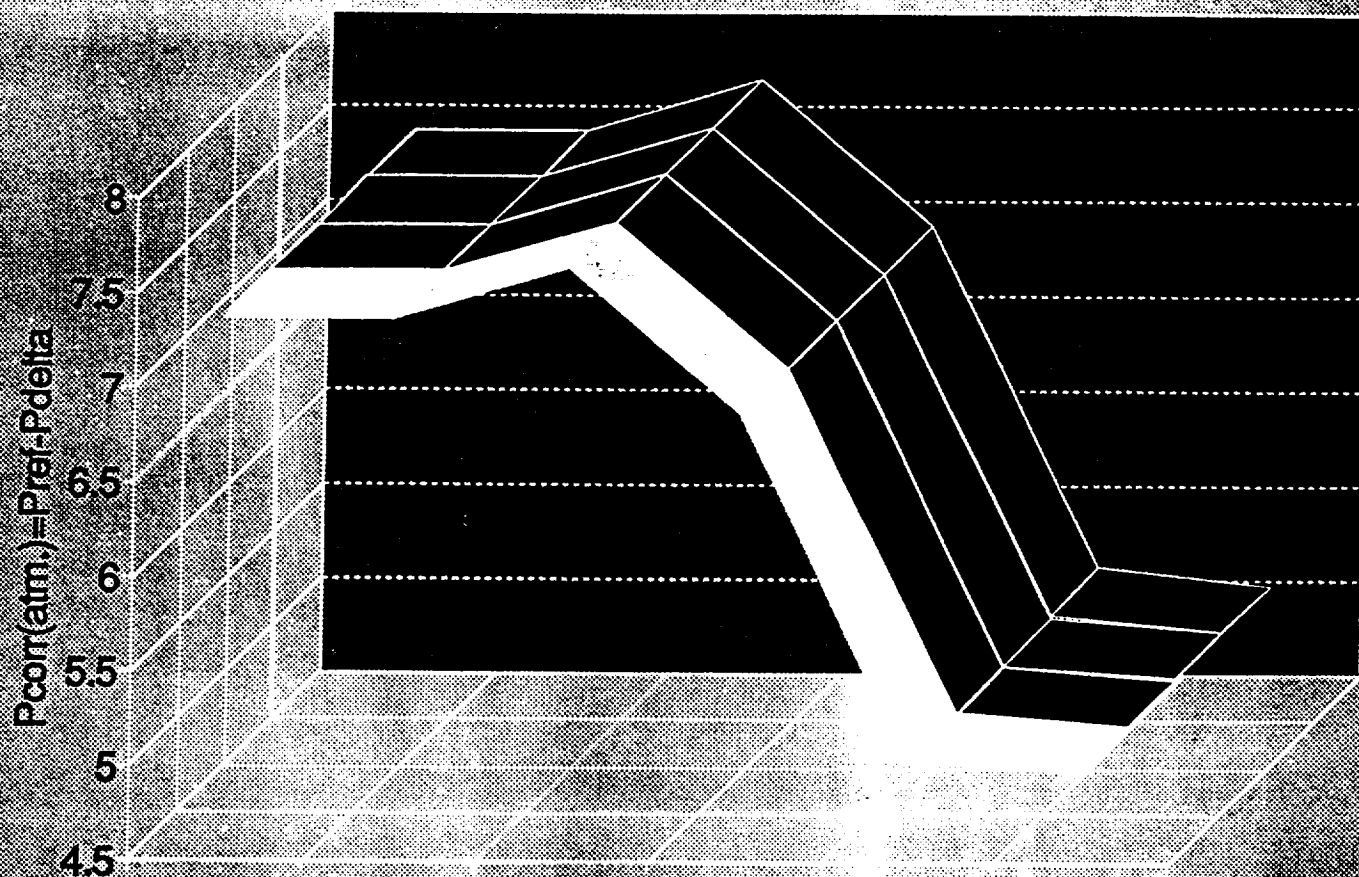


Position: I=2 to 8 by 2, J=2 to 12 by 2



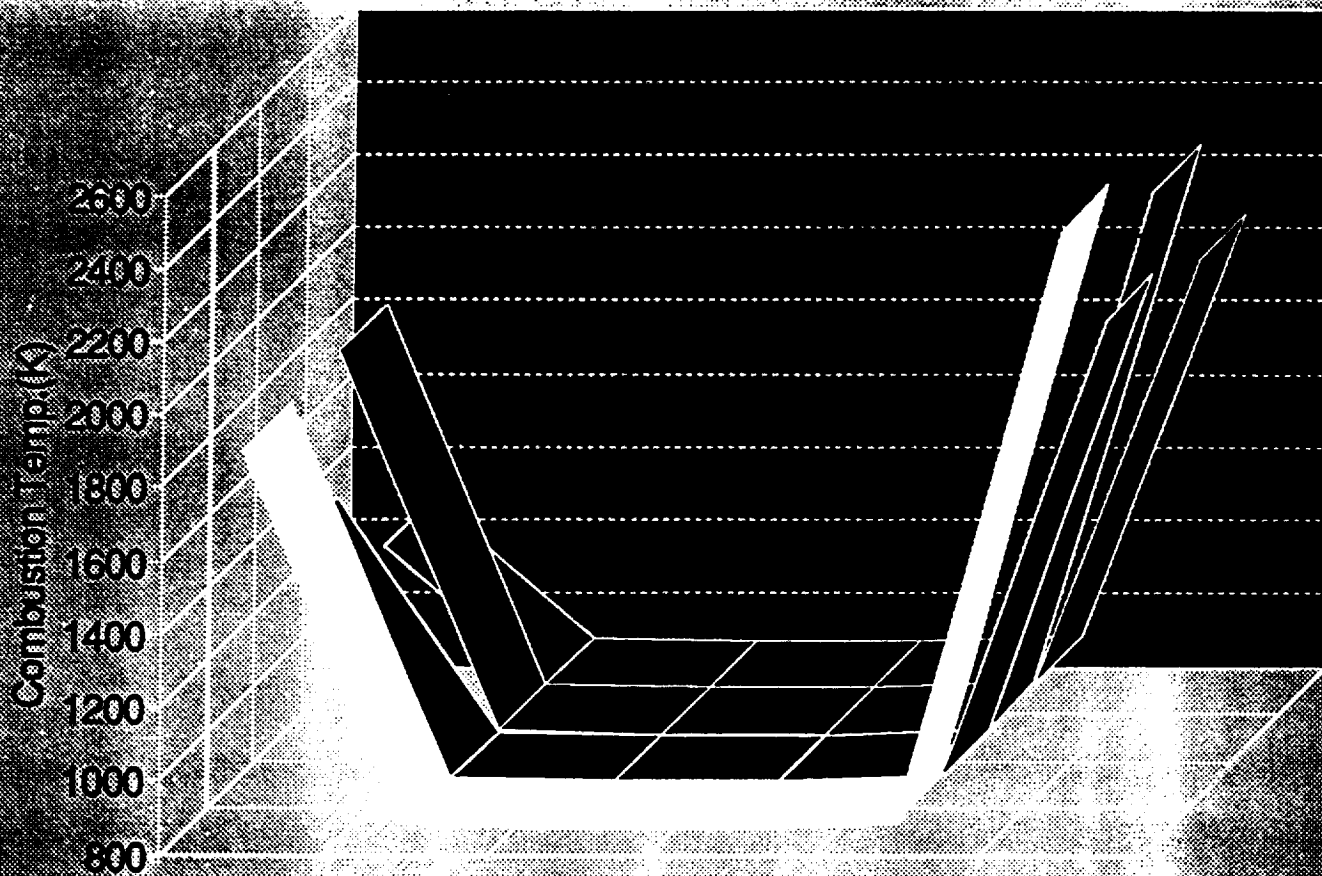
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# PRESSURE



Position:  $I=2$  to  $8$  by  $2$ ,  $J=2$  to  $12$  by  $2$

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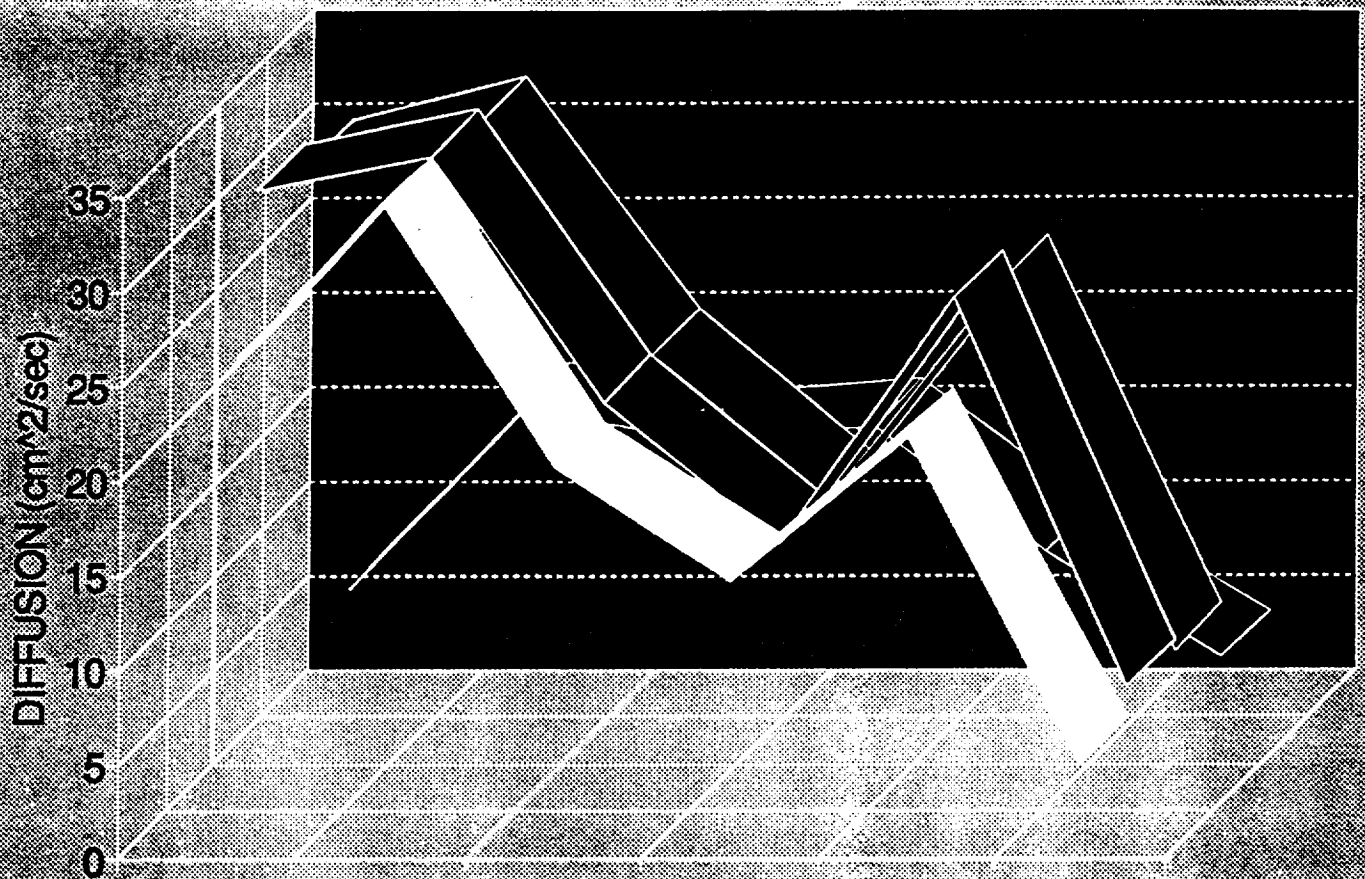


Position: I=2to8by2, J=2to12by2



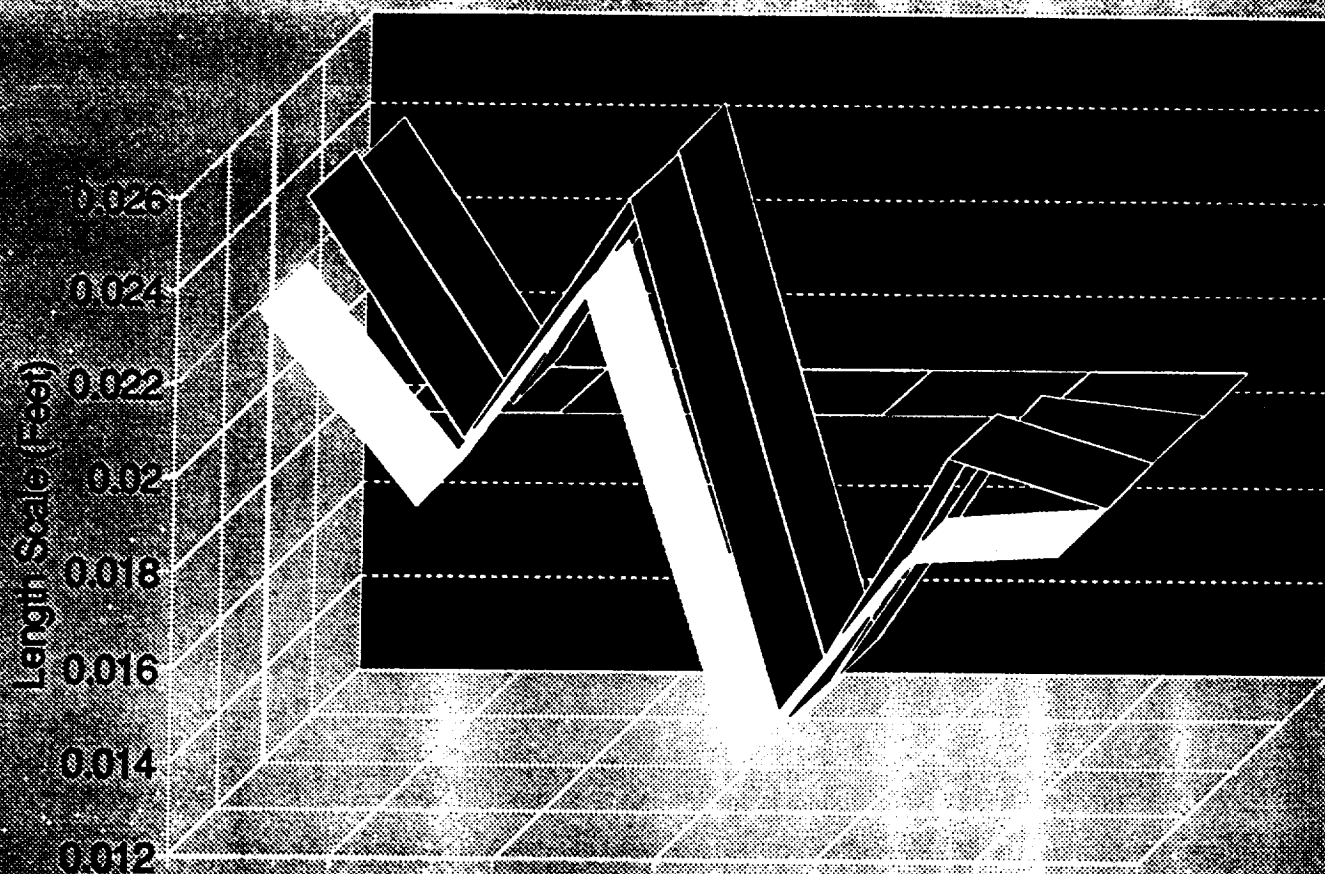
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# MASS DIFFUSIVITY OF OXYGEN



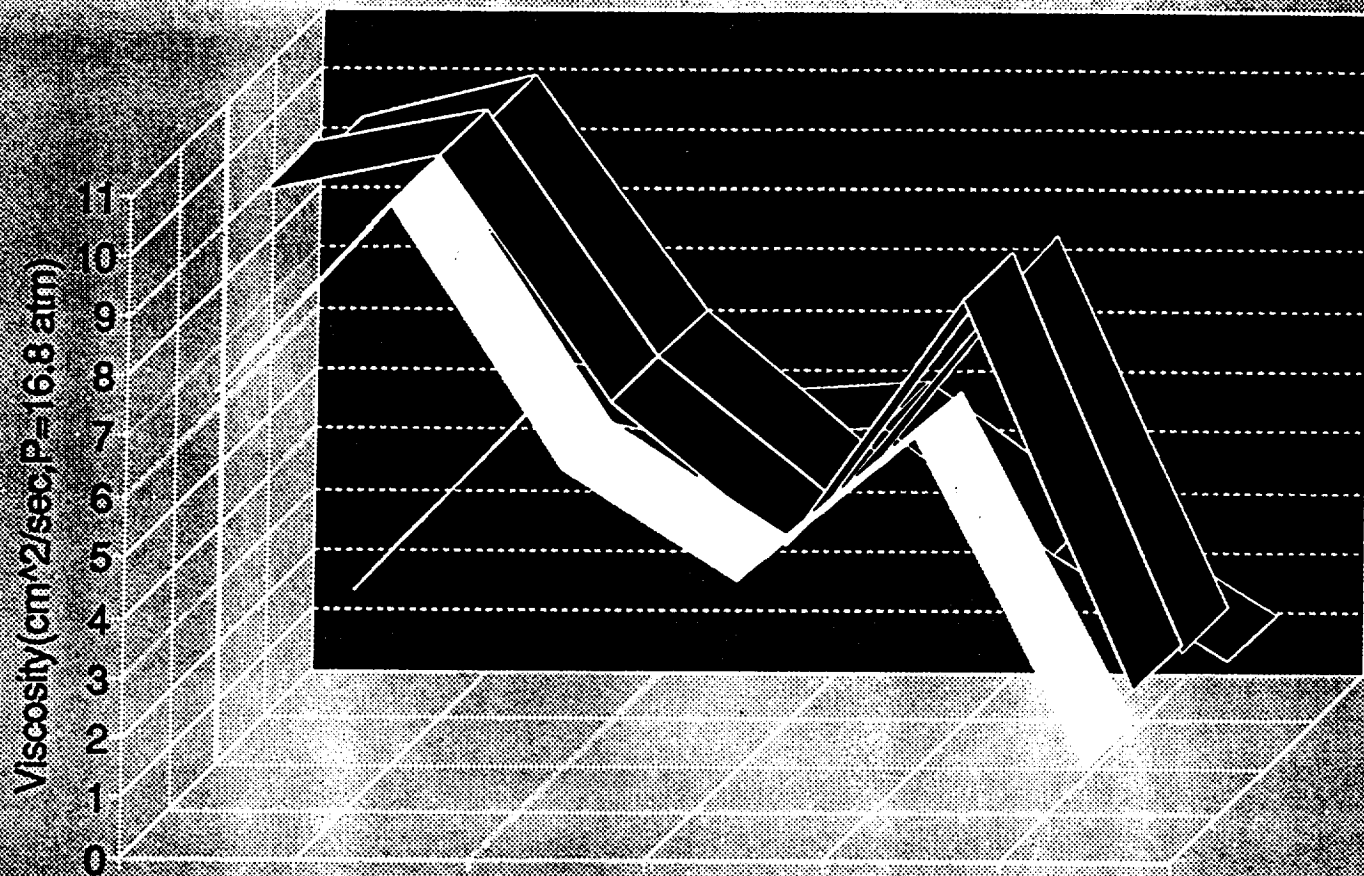
Position: I=2 to 8 by 2, J=2 to 12 by 2

# KOLMOGOROV LENGTH SCALE



Position: I=2 to 8 by 2, J=2 to 12 by 2

# KINEMATIC VISCOSITY



Position:  $I=2$  to  $8$  by  $2$ ,  $J=2$  to  $12$  by  $2$

## MIXING TIME OF O<sub>2</sub>( $t_{\text{bar}}=.00375$ )

